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14. ABSTRACT Equilibrium and nonequilibrium molecular dynamics (MD) implemented on parallel processing computers was used to simulate supercritical fuel phenomena occurring in high pressure combustion devices. The coefficients of diffusion, viscosity and thermal conductivity and the equation of state of argon, oxygen, nitrogen and various alkanes at high pressures and temperatures were obtained via molecular dynamics with the obtained values agreeing with and extending NIST SUPERTRAPP code values. The hydrocarbons ethylene, butane and pentane were simulated. Vibrational energy, dissociation and recombination in oxygen and hydrogen diatomic molecules were simulated with the computed high temperature dissociation rates in agreement with published experimental measurements.					
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## FINAL REPORT

### MOLECULAR DYNAMICS INVESTIGATION OF SUPERCRITICAL FUELS

AFOSR Grant No. F49620-97-1-0128

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#### ABSTRACT

Equilibrium and nonequilibrium molecular dynamics (MD) implemented on parallel processing computers was used to simulate supercritical fuel phenomena occurring in high pressure combustion devices. The coefficients of diffusion, viscosity and thermal conductivity and the equation of state of argon, oxygen, nitrogen and various alkanes at high pressures and temperatures were obtained via molecular dynamics with the obtained values agreeing with and extending NIST SUPERTRAPP code values. The hydrocarbons ethylene, butane and pentane were simulated. Vibrational energy, dissociation and recombination in oxygen and hydrogen diatomic molecules were simulated with the computed high temperature dissociation rates in agreement with published experimental measurements.

#### TECHNICAL SUMMARY

Transport Properties and Equation of State. Molecular dynamics has been used to calculate the coefficients of diffusion, viscosity and thermal conductivity and the equation of state of pure oxygen, nitrogen, ethylene, butane, pentane and hexane at high (supercritical) pressures and temperatures<sup>1,2</sup>. The transport coefficients are obtained by one of several methods. Equilibrium molecular dynamics (EMD) computes the transport coefficients by calculating the autocorrelation functions for a system in equilibrium<sup>3</sup>. This requires the computation of the autocorrelation functions over very long time periods in order to obtain accurate results. The shear viscosity coefficient measures the resistance of the fluid to a shearing force. For the shear viscosity the integration is over the non-diagonal terms of the stress tensor and it is a collective property of the fluid. The Green-Kubo formula is given by,

$$\mu_{xy} = \frac{1}{Vk_b T} \int_0^{\infty} \langle J^{xy}(t_0) J^{xy}(t_0 + t) \rangle dt \quad (1)$$

where  $J^{xy}$ , an off-diagonal term of the stress tensor, is given by

$$J^{xy} = m \sum_{i=1}^N v_i^x v_i^y - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N r_{ij}^x \nabla_y \Phi(r_{ij}) \quad (2)$$

Here  $T$  and  $V$  denote the temperature and volume of the system, respectively, and  $m$  denotes the mass of each particle.  $v^x$ ,  $r_{ij}$  and  $\Phi(r_{ij})$  denote the  $x$ -direction velocity, position vector and the potential, respectively, between particles  $i$  and  $j$ . Statistical precision is improved by averaging over all six terms that result from the stress tensor:

$$\mu = \frac{1}{6} (\mu_{xy} + \mu_{yx} + \mu_{xz} + \mu_{zx} + \mu_{yz} + \mu_{zy}) \quad (3)$$

The thermal conductivity coefficient measures the transport of heat in a system. The correlation function is obtained from the heat current and it is also a collective property of the entire fluid. The Green-Kubo formula is given by:

$$\lambda_x = \frac{1}{Vk_b T^2} \int_0^\infty \langle T_q^x(t_0) T_q^x(t_0 + t) \rangle dt \quad (4)$$

where  $T_q^x$  denotes an arbitrary component of the heat current and is given by

$$T_q^x = \frac{m}{2} \sum_{i=1}^N |v_i|^2 v_i^x - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left[ (r_{ij}^x \nabla_x \Phi(r_{ij}) - \Phi(r_{ij})) i \right] v_i \quad (5)$$

where  $i$  denotes a unit tensor. Again, statistical precision is improved by averaging over all three components:

$$\lambda = \frac{1}{3} (\lambda_x + \lambda_y + \lambda_z) \quad (6)$$

These functions are computed during the simulation. The velocity autocorrelation is computed outside the force subroutine, while the other components of the other autocorrelation functions are calculated within it. Once the correlation functions have been obtained, standard numerical integration techniques are used to obtain the transport coefficients. The statistical precision of the self-diffusion coefficient is improved by averaging over all the particles in the system. The viscosity and thermal conductivity values are improved by averaging over all the six terms from the stress tensor, and the three terms of the heat current, respectively. Figures 1 and 2 compare the MD calculated coefficients of viscosity and thermal conductivity for ethylene at 10 MPa and a range of temperatures with NIST Database 4 (SUPERTRAPP) provided values<sup>4</sup>. Figures 3 and 4 show the MD calculated coefficients of viscosity and thermal conductivity for butane at 50 MPa and Figures 5 and 6 show the MD calculated coefficients of viscosity and thermal conductivity for pentane at 50 MPa. The calculated values agree well with the NIST values over the temperature range examined (300-600 K) for these high supercritical pressures.

When the calculations proceeded to hexane the computation times for the viscosity and the thermal conductivity autocorrelations became excessive. Nonequilibrium molecular dynamics (NEMD) can be used to calculate the transport coefficients using less computation time but with greater algorithm complexity<sup>5</sup>. NEMD applies a force, either diffusive, momentum or energy, to a system and the rate of transport of the desired quantity is computed. In order to compute the viscosity we considered the case of Couette flow in which the fluid undergoes sheared flow due to boundary walls that are in relative motion. The usual microscopic definition of temperature in terms of mean-square velocity assumes that there is no overall motion; any local flow must be subtracted from the velocities before using them to evaluate temperature. The same holds true for the velocities used in the thermostat. However, knowing the bulk flow to an accuracy suitable for use in the equations of motion implies that the problem has already been solved; this circularity can be removed by assuming the nature of the flow, and only later checking to see whether consistent results are obtained. A less reliable alternative is to evaluate local flow by means of coarse-grained averaging, and then use the results in the equations of motion. Such an approach is unstable to any fluctuations in the flow because these variations are interpreted by the equations of motion as temperature fluctuations that must be suppressed.

In this work we imposed the reasonable requirement that the MD flow obeys the linear velocity profile known from the exact solution of the continuum problem. Assuming it is the z-boundaries that are in motion, then if the relative velocity of the walls is  $\gamma L_z$ , the shear rate  $dv_x/dz$  has the constant value  $\gamma$ . The thermostatic equation of motion is then,

$$\ddot{\mathbf{r}}_i = \mathbf{F}_i/m + \alpha(\dot{\mathbf{r}}_i - \gamma z_i \mathbf{x}) \quad (7)$$

Where  $\mathbf{x}$  is a unit vector in the x-direction, and  $\mathbf{r} = \mathbf{r}(x, y, z)$  is the position vector. The value of the Lagrange multiplier  $\alpha$  follows from the constant temperature constraint:

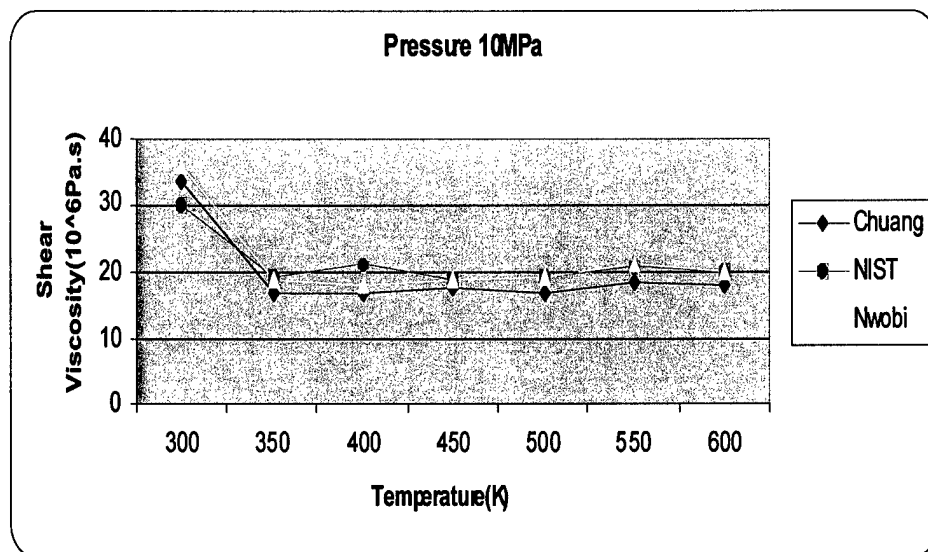


Figure 1. Shear viscosity for ethylene  $C_2H_2$ ,  $P = 10$  MPa.

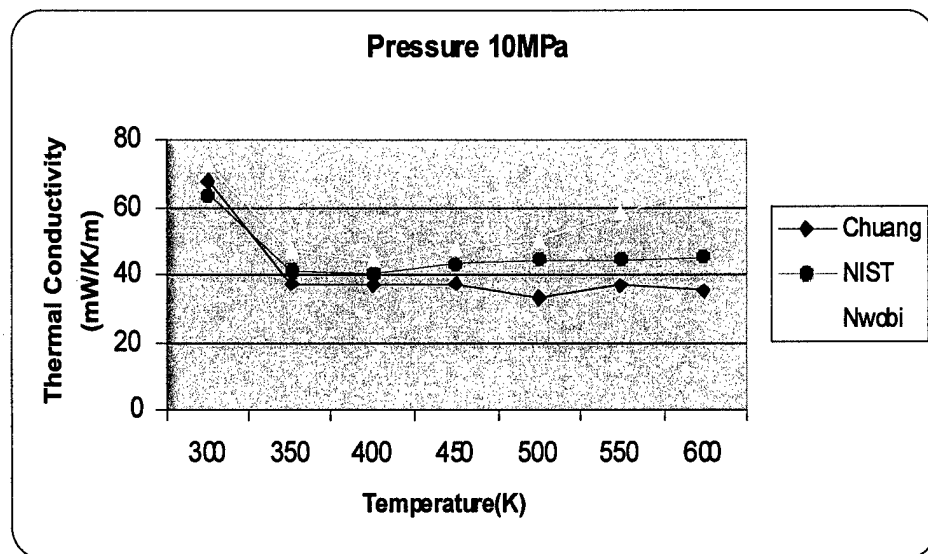


Figure 2. Thermal conductivity of ethylene  $C_2H_2$ ,  $P = 10$  MPa.

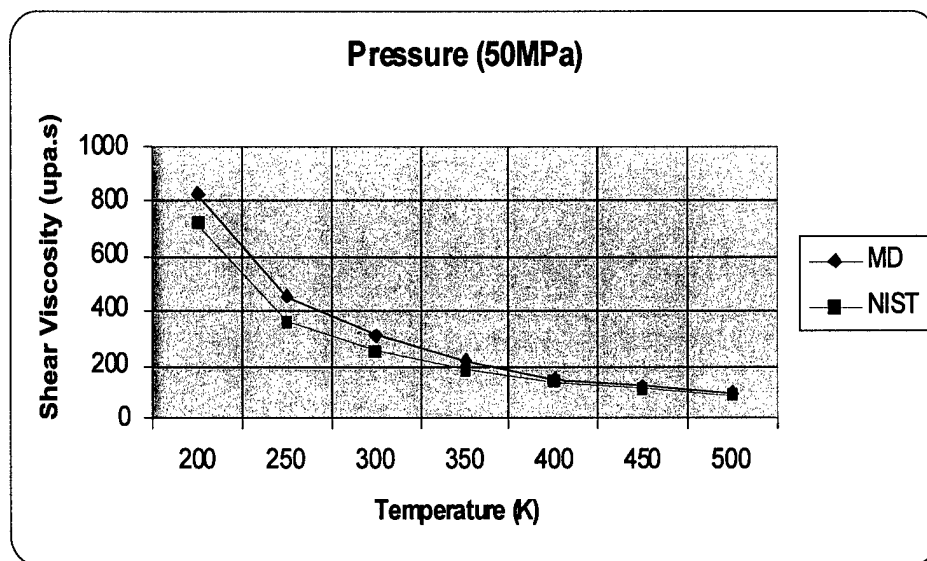


Figure 3. Shear viscosity of butane  $C_4H_{10}$ ,  $P=50$  MPa.

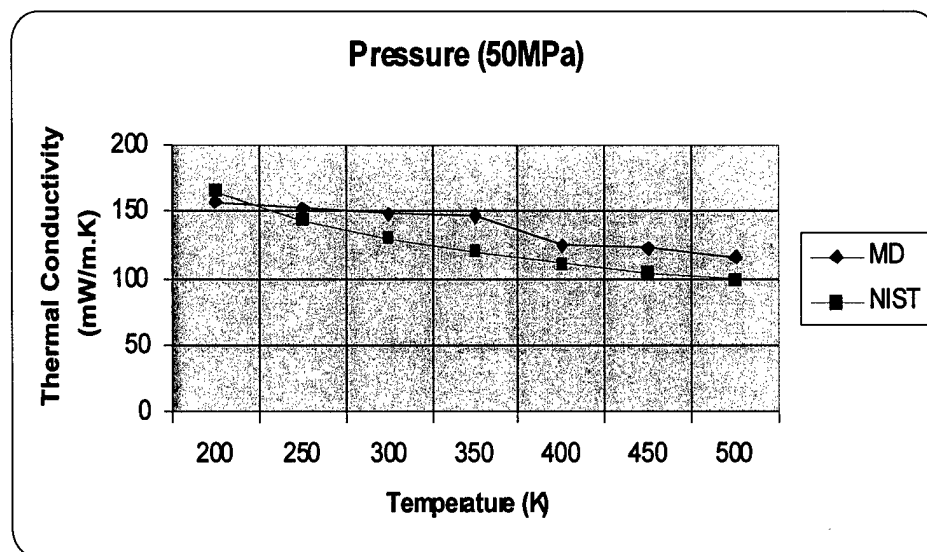


Figure 4. Thermal conductivity of butane  $C_4H_{10}$ ,  $P=50$  MPa.

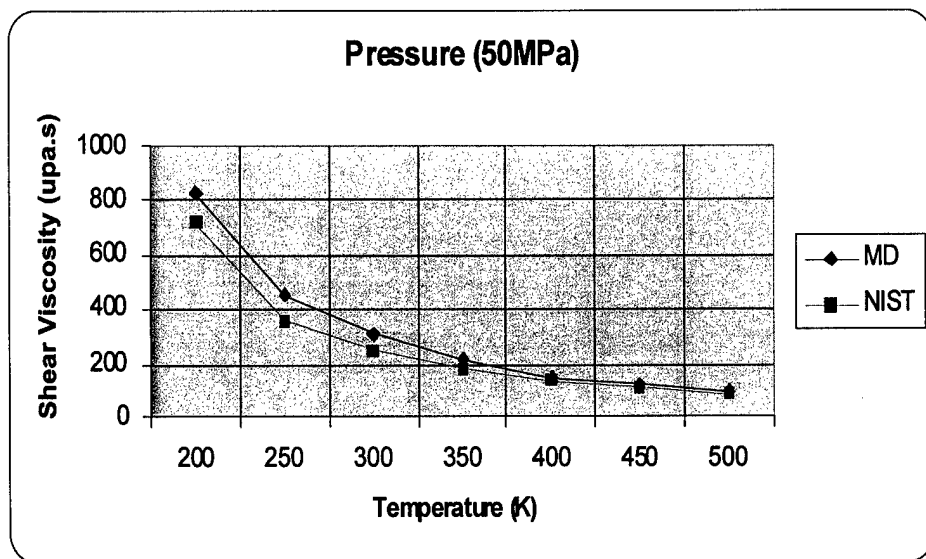


Figure 5. Shear viscosity of pentane  $C_5H_{10}$ ,  $P = 50$  MPa.

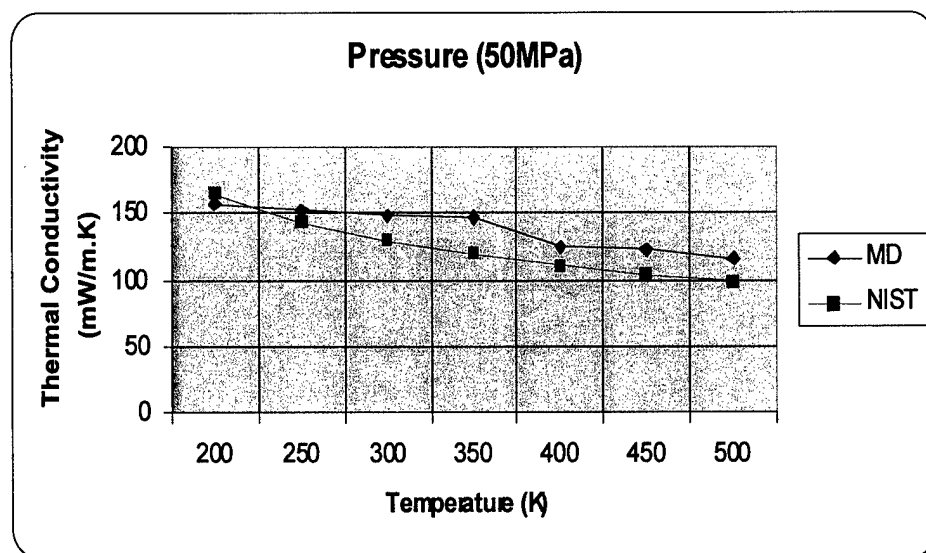


Figure 6. Thermal conductivity of pentane  $C_5H_{10}$ ,  $P = 50$  MPa.

$$\alpha = - \frac{\sum_i (\dot{\mathbf{r}}_i - \gamma \mathbf{r}_{zi} \mathbf{x}) \cdot (\mathbf{F}_i / m - \gamma \mathbf{r}_{zi} \mathbf{x})}{\sum_i (\dot{\mathbf{r}}_i - \gamma \mathbf{r}_{zi} \mathbf{x})^2} \quad (8)$$

The equation (8) assumes that the linear velocity profile has already been established. Creating the initial sheared flow is most readily done as part of the initial conditions, and from the more formal point of view this amounts to applying an impulse of the correct size and direction to each atom at  $t = 0$ . The sliding boundaries, in the form of a special type of boundary condition, maintain the constant shear rate. The constant temperature version of linear response theory for this problem provides an expression for  $\eta$  based on the pressure tensor,

$$\eta = - \lim_{\gamma \rightarrow 0} \lim_{t \rightarrow \infty} \langle P_{xz} \rangle / \gamma \quad (9)$$

Defining the momentum measured relative to the local flow  $\mathbf{p}_i / m = \dot{\mathbf{r}}_i - \gamma \mathbf{r}_{zi} \mathbf{x}$ , the first-order equations are then

$$\dot{\mathbf{r}}_i = \mathbf{p}_i / m + \gamma \mathbf{r}_{zi} \mathbf{x} \quad (10)$$

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \gamma \mathbf{p}_{zi} \mathbf{x} + \alpha \mathbf{p}_i \quad (11)$$

The boundaries are periodic, but of a special form to accommodate the uniformly sheared flow. The idea is to replace sliding walls by sliding replica systems: layers of replicas that are adjacent in the  $z$ -direction move with a relative velocity  $\gamma L_z \mathbf{x}$ , an arrangement designed to ensure periodicity at shear rate  $\gamma$ . An atom crossing a  $z$ -boundary requires special treatment because the  $x$ -components of position and velocity are both discontinuous (not for the replica system just entered but relative to the opposite side of the region itself into which the atom is actually inserted). The velocity change whenever a  $\pm z$  boundary is crossed is  $\mp \gamma L_z \mathbf{x}$ , and the coordinate change is  $\mp d_x \mathbf{x}$ , where the total relative displacement of the neighboring replicas - only meaningful over the range  $(-L_x/2, L_x/2)$  - is given by

$$d_x = (\gamma L_z t + L_x / 2) \bmod L_x - L_x / 2 \quad (12)$$

Note that because the  $x$ -coordinate changes when a  $z$ -boundary is crossed, and additional correction for periodic wraparound in the  $x$ -direction may be needed. Interactions that occur between atoms separated by the  $z$ -boundary require an offset value  $-d_x$  to be included in the distance computation.

To simulate the thermal conductivity, a fictitious external field  $\mathbf{F}_e$  of a rather unusual kind is introduced. It has the effect of driving atoms with a higher than average energy in the direction of  $\mathbf{F}_e$ , while those with a lower energy are driven to the opposite direction. In other words  $\mathbf{F}_e$  generates heat flow and so, at least for small values of the field, produces the effect of an imposed temperature difference.

The additional force acting on each atom is defined as,

$$\mathbf{F}'_i = e_i \mathbf{F}_e + \frac{1}{2} \sum_{j \neq i} \mathbf{f}_{ij} (\mathbf{r}_{ij} \cdot \mathbf{F}_e) - \frac{1}{2 N_a} \sum_{j \neq k} \mathbf{f}_{jk} (\mathbf{r}_{jk} \cdot \mathbf{F}_e) \quad (13)$$

where,

- $e_i$  The excess energy of atom  $i$  over average,  $e_i = \frac{1}{2} m v_i^2 + \frac{1}{2} \sum_{i \neq j} u(r_{ij}) - \langle e \rangle$ ;
- $\langle e \rangle$  The mean energy;
- $u(r_{ij})$  Lennard-Jones potential energy;
- $\mathbf{F}_e$  The fictitious external force;

- $\mathbf{f}_{ij}$  The force between atom  $i$  and  $j$  based on Lennard-Jones Potential model;  
 $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ ;  
 $N_a$  The total number of atoms;  
 $\mathbf{F}_i'$  The additional force acting on atom  $i$ ;

Here  $\mathbf{F}_i'$  has been chosen so that in terms of the heat current  $S$  is,

$$\sum_i \dot{\mathbf{r}}_i \cdot \mathbf{F}_i' = VS \cdot \mathbf{F}_e \quad (14)$$

where  $S$  is,

$$S = \frac{1}{V} \left[ \sum_j e_j \mathbf{v}_j + \frac{1}{2} \sum_{i \neq j} \mathbf{r}_{ij} (\mathbf{f}_{ij} \cdot \mathbf{v}_j) \right] \quad (15)$$

- $V$  Volume of the system,  $V = N_a / n$ ;  
 $n$  Number density, number of atoms per unit volume  
 $\mathbf{v}_j$  Velocity of atom  $j$

The force conserves total momentum because  $\sum \mathbf{F}_i' = 0$ , since only relative distances occur in  $\mathbf{F}_i'$ , and assuming the force is sufficiently weak that the system remains homogeneous, there is nothing to prevent the use of periodic boundary conditions, exactly the motivation for devising methods of this kind. If  $J = S_z$ , and  $\mathbf{F}_e = F_e \mathbf{z}$ , then the constant temperature version of  $Q = \lim_{F_e \rightarrow 0} \lim_{t \rightarrow \infty} \langle J(t) \rangle / F_e$  leads to

$$\lambda = \lim_{F \rightarrow 0} \lim_{t \rightarrow \infty} \frac{\langle S_z \rangle}{F_e T} \quad (16)$$

The thermostat is the usual one, based on the total force, so that the equations of motion are simply

$$\ddot{\mathbf{r}}_i = \mathbf{F}_i + \mathbf{F}_i' + \alpha \dot{\mathbf{r}}_i \quad (17)$$

Since the applied force  $F_e$  performs mechanical work on the system the temperature rises, and equilibrium is never attained. To eliminate this problem a thermostat is included in the dynamics by adding a term  $\alpha \mathbf{p}_i$  to the variation rate of momentum of every atom; constant kinetic energy is assured if the value of the Lagrange multiplier is

$$\alpha = \frac{\sum_i \left[ \mathbf{F}_i + e_i \mathbf{F}_e + \frac{1}{2} \sum_{j \neq i} \mathbf{f}_{ij} (\mathbf{r}_{ij} \cdot \mathbf{F}_e) - \frac{1}{2N_a} \sum_{j \neq k} \mathbf{f}_{jk} (\mathbf{r}_{jk} \cdot \mathbf{F}_e) \right] \cdot \mathbf{p}_i}{\sum_i \mathbf{p}_i^2} \quad (18)$$

where  $\mathbf{p}_i$  is the momentum of atom  $i$ ,  $\mathbf{p}_i = m \mathbf{v}_i$ .

NEMD simulations were conducted for argon and ethylene before the grant period ended. Figure 7 plots the thermal conductivity of ethylene as a function of temperature at 5 MPa pressure. Excellent agreement between NEMD and NIST SUPERTRAPP results can be seen, especially at the higher temperature.

The fluid pressure for a given temperature and density is calculated from the virial coefficients. Figure 8 compares MD calculated pressures for ethylene with experimental data<sup>5</sup>. Agreement is good except at the highest density, which could be improved by using better interatomic potentials.



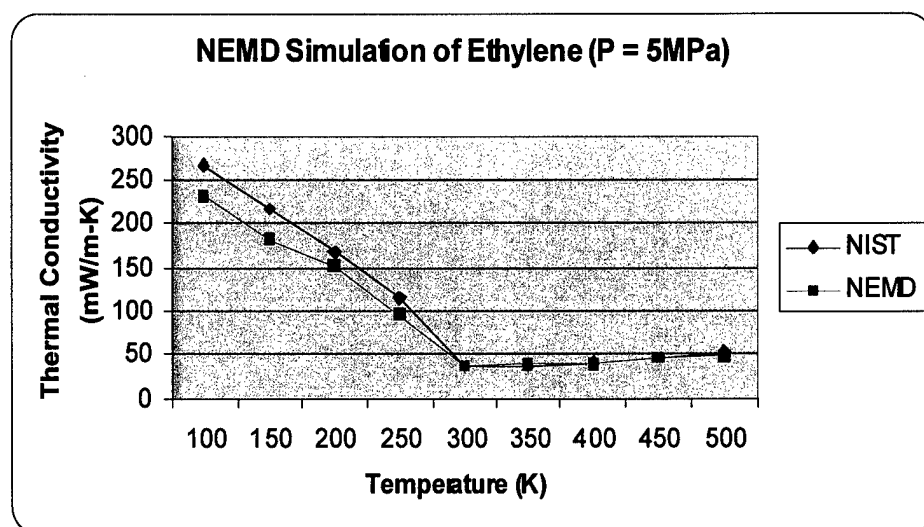


Figure 7. NEMD simulation of thermal conductivity of ethylene  $C_2H_2$ ,  $P=5MPa$ .

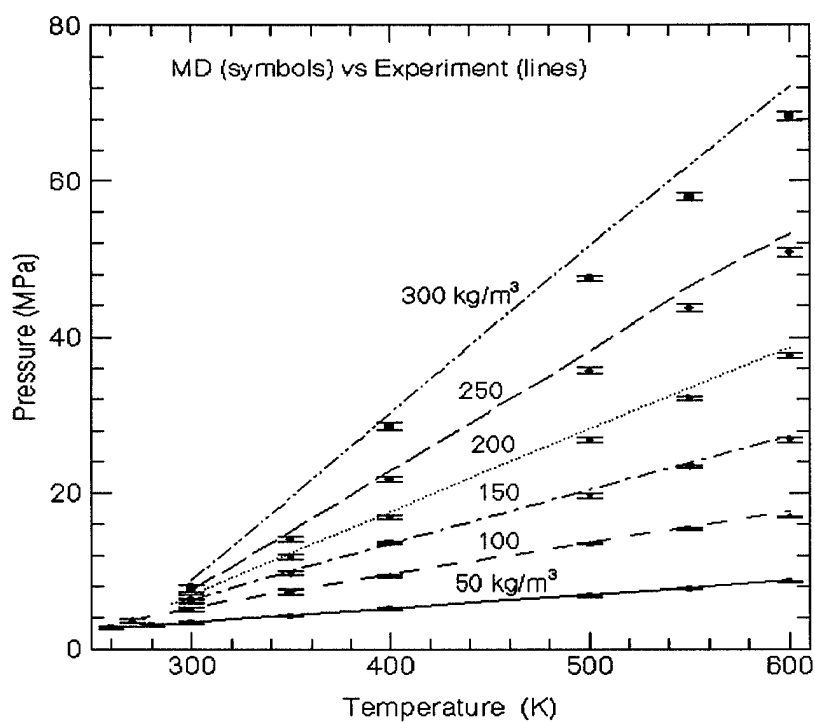


Figure 8. Ethylene MD equation of state calculations compared to experimental data.

Vibrational Energy and Dissociation. As a first step towards modeling chemical reactions, the vibrational motions and excitation of diatomic oxygen and the subsequent dissociation were directly simulated using molecular dynamics<sup>6</sup>. The Morse potential<sup>7</sup> is used to determine the internuclear force between the two atoms bound in the molecule

$$V(r) = De^{-2\beta(r-r_c)} - 2De^{-\beta(r-r_c)} + E_\infty \quad (19)$$

where  $D$  is the dissociation energy,  $r$  is the internuclear separation,  $r_c$  is the mean bond length, and  $E_\infty$  and  $\beta$  are constants computed from spectroscopic data. Atomic interactions outside the molecule are modeled using the Lennard-Jones potential. For a given temperature and density, the MD calculated vibrational energy distribution at equilibrium demonstrated excellent agreement with the Boltzmann distribution.

Dissociation is simulated by monitoring the potential energy between the two vibrating atoms in a molecule. When the potential energy exceeds a critical value due to increased separation between the two atoms, dissociation is judged to occur and the Morse potential between the two atoms is removed<sup>8-10</sup>. Recombination is also possible by the reverse mechanism. This process enables a system to start in a state of oxygen molecules and proceed to an equilibrated state of atomic and molecular oxygen. Figure 9 shows the rate of oxygen dissociation from a single unensembled molecular dynamics computation using 108 molecules compared to that predicted by kinetic theory<sup>11</sup> using experimentally determined parameters<sup>12,13</sup> at a temperature of 6344 K. Excellent agreement between the two for both the rate of dissociation and the final equilibrium value is shown.

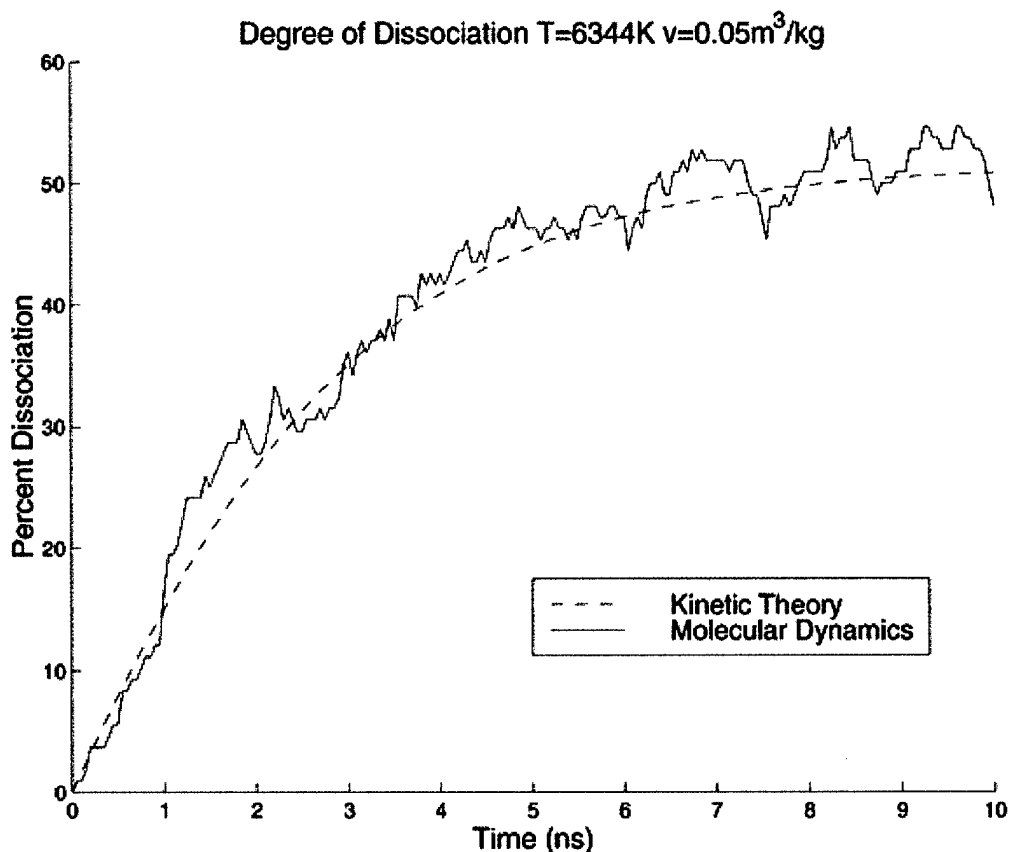


Figure 9. MD calculated oxygen dissociation rate compared to kinetic theory prediction.

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## PERSONNEL

### Professional Staff

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### Graduate Students

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Chuang Li

## PUBLICATIONS

Kaltz, T. L., Long, L. N., Micci, M. M. and Little, J. K., "Supercritical Vaporization of Liquid Oxygen Droplets Using Molecular Dynamics," *Combustion Science and Technology*, Vol. 136, Nos. 1-6, 1998, pp. 279-301.

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Obika C. Nwobi, *Molecular Dynamics Studies of Transport Properties and Equation of State of Supercritical Fluids*, Ph.D. Thesis, The Pennsylvania State University, December 1998.

Andrew Kantor, *Molecular Dynamics Simulation of Dissociation Kinetics*, M.S. Thesis, The Pennsylvania State University, December 1999.

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## HONORS/AWARDS

Best Paper Award for "Molecular Dynamic Modeling of Supercritical LOX Evaporation" by Kaltz, Long and Micci. Presented by the American Institute of Aeronautics and Astronautics Liquid Propulsion Technical Committee, July 1998.

## PRESENTATIONS AND INTERACTIONS

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Kantor, A. L., Long, L. N. and Micci, M. M., "Molecular Dynamics Simulation of Dissociation Kinetics." Presented at the 38<sup>th</sup> Aerospace Sciences Meeting, Reno, NV, Jan. 10-13, 2000.

12 JUN 2000

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**PI DATA**

Name (Last, First, MI) Micci, Michael M. and Long, Lyle N.

Institution The Pennsylvania State University

Contract/Grant No F49620-97-1-0128

**AFOSR USE ONLY**

Project/Subarea

\_\_\_\_\_/\_\_\_\_

NX \_\_\_\_\_

FY \_\_\_\_\_

**NUMBER OF CONTRACT/GRANT CO-INVESTIGATORS**

Faculty 2

Post Doctorates \_\_\_\_\_

Graduate Students 4

Other \_\_\_\_\_

**PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT**

**NOTE:** List names in the following format: Last Name, First Name, MI

**Include:** Articles in peer reviewed publications, journals, book chapters, and editorships of books.

**Do Not Include:** Unreviewed proceedings and reports, abstracts, "Scientific American" type articles, or articles that are not primary reports of new data and articles submitted or accepted for publication, but with a publication date outside the stated time frame.

Name of Journal, Book, etc: Journal of Thermophysics and Heat Transfer

Title of Article: Molecular Dynamics Studies of Properties of Supercritical Fluids

Author(s): Nwobi, Obika C., Long, Lyle N. and Micci, Michael M.

Publisher (if applicable): American Institute of Aeronautics and Astronautics

Volume: 12 Page(s): 322-327 Month Published: July-Sept. Year Published: 1998

Name of Journal, Book, etc: Combustion Science and Technology

Title of Article: Supercritical Vaporization of Liquid Oxygen Droplets Using Molecular Dynamics

Author(s): Kaltz, Terri L., Long, Lyle N., Micci, Michael M. and Little, Jeffrey K.

Publisher (if applicable): Gordon and Breach Science

Volume: 136 Page(s): 279-301 Month Published: July Year Published: 1998

Name of Journal, Book, etc Proceedings of the 11st International Symposium on Rarefied Gas Dynam

Title of Article Molecular Dynamics Simulation of Oxygen Droplet Vaporization

Author(s) Kaltz, Teresa L., Long, Lyle N. and Micci, Michael M.

Publisher (if applicable) Cepadues-Editions, Toulouse, France

Volume I Page(s) 543-550 Month Published July Year Published 1999

Name of Journal, Book, etc Journal of Thermophysics and Heat Transfer

Title of Article Molecular Dynamics Studies of Thermophysical Properties of Supercritical Ethyle

Author(s) Nwobi, Obika C., Long, Lyle N. and Micci, Michael M.

Publisher (if applicable) American Institute of Aeronautics and Astronautics

Volume 13 Page(s) 351-354 Month Published July-Sept. Year Published 1999

#### HONORS/AWARDS RECEIVED DURING CONTRACT/GRANT LIFETIME

Include: All honors and awards received during the lifetime of the contract or grant, and any life achievement honors such as (Nobel prize, honorary doctorates, and society fellowships) prior to this contract or grant.

Do Not Include: Honors and awards unrelated to the scientific field covered by the contract/grant.

Honor/Award Best Paper Award Year Received: 1998

Honor Award Recipient(s) Teresa L. Kaltz, Lyle N. Long and Michael M. Micci

Awarding Organization American Institute of Aeronautics and Astronautics